5-Pregnen-3«beta»-ol-20-one, formate

Inchi: InChI=1S/C22H32O3/c1-14(24)18-6-7-19-17-5-4-15-12-16(25-13-23)8-10-21(15,2)20(17
InchiKey: PMKWQPYDHKLDTD-UHFFFAOYSA-N
Formula: C22H32O3
SMILES: CC(=O)C1CCC2C3CC=C4CC(OC=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 344.49

Physical Properties

Property code	Value	Unit	Source
gf	-30.36	kJ/mol	Joback Method
hf	-551.62	kJ/mol	Joback Method
hfus	31.30	kJ/mol	Joback Method
hvap	78.68	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.696		Crippen Method
mcvol	282.110	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	2412.00		NIST Webbook
rinpol	2412.00		NIST Webbook
tb	866.63	K	Joback Method
tc	1102.62	K	Joback Method
tf	554.38	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.32	J/mol×K	866.63	Joback Method
cpg	1018.21	J/mol×K	905.96	Joback Method
cpg	1044.10	J/mol×K	945.29	Joback Method
cpg	1070.34	J/mol×K	984.63	Joback Method
cpg	1097.28	J/mol×K	1023.96	Joback Method
cpg	1125.23	J/mol×K	1063.29	Joback Method
cpg	1154.55	J/mol×K	1102.62	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368370&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume